Gain and loss enhancement of passive and active materials in a square periodic array of cylinders

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Summary
The asymptotic homogenization method is applied to complex dielectric two-phase fibrous composites. Under continuity conditions at the interfaces, we derive closed-form formulas for the complex dielectric effective tensor in the case of isotropic non-overlapping circular inclusions embedded in an isotropic square matrix. These formulas are given in terms of a symmetrical matrix which facilitates the implementation of the computational scheme, and are advantageous for estimating gain and loss enhancement properties of active and passive fibrous composites. Numerical computations are performed in order to find the regions where enhancement properties are guaranteed. This study may be of interest in the context of metamaterials.

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1. Introduction

The fundamental problem of finding the overall behavior of such heterogeneous media in material sciences has been intensely investigated during the last few years. For instance, in [1], based on the asymptotic homogenization method and solving the corresponding local problems using Weierstrass elliptic functions, a simple analytical expression is derived for the effective complex conductivity of a periodic hexagonal arrangement of conductive circular cylinders embedded in a conductive matrix, with interfaces exhibiting capacitive impedance. In [2], based on series expansions of Weierstrass ζ-function and its derivatives, efficient formulas are obtained for computing the effective complex permittivity tensor of two-dimensional periodic dielectric composites consisting of an arbitrary doubly periodic array of identical circular cylinders in a homogeneous matrix. The results of [2] have been applied in [3], to acoustics showing a good agreement with experimental results and inertial enhancement. In [4], the results of [2] are used for calculate eddy current losses in soft complex magnetic composites. A complex variable method is also developed in [5] to evaluate the transverse effective transport properties of composites with a doubly-periodic fiber array. The obtained complex variable solution is derived in an unified form for the arbitrary doubly periodic fiber array, and different fiber-matrix interfaces, i.e., perfect interface, contact resistance interface and coating. Here, the study of the effective behavior of complex dielectric composites is done by the homogenization of the equivalent system of equations with real coefficients. By using previous results [6], closed-form formulas for the effective coefficients are obtained and employed to study gain-enhancement (GE) and loss-enhancement (LE) properties of the homogenized material. The closed-form formulas are explicitly given and depend on a $2n_0 \times 2n_0$ symmetric matrix, where n_0 indicates the truncation order. Particularly, a parametrical study is done in order to find the regions where enhancement properties are guaranteed by using the sufficient conditions given in [7]. Within the realm of metamaterials the results of this study maybe useful as in [8].

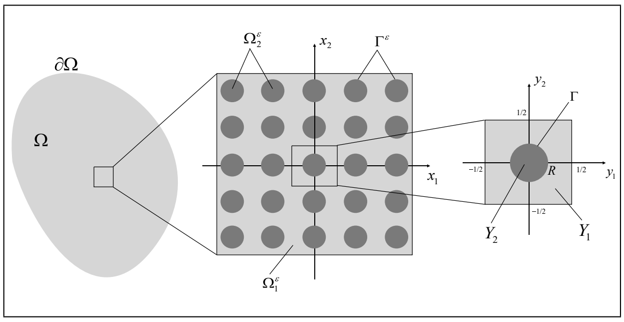

Figure 1. (Left) A blow-up domain contained in Ω showing (Center) a FRC type of geometry in global coordinates. (Right) Square unit cell in y-coordinates.

2. Problem statement

Let us consider a fiber-reinforced composite with cross-section $\Omega \subset \mathbb{R}^2$ and sufficiently smooth boundary $\partial\Omega$. Let ε be a small geometric parameter characterizing the micro-structure so that, the scaled local or fast coordinates $\boldsymbol{y} = \boldsymbol{x}/\varepsilon$ are introduced where $\boldsymbol{x} = (x_1, x_2)$ represent the global or slow coordinates. The periodic square unit cell cross-section is $Y \subset \mathbb{R}^2$, where Y_1 and Y_2 denote the matrix and the circular fiber of radius R, respectively (Fig. 1).

We assume that the constituents Ω_1^ε and Ω_2^ε of the composite medium represent two materials that have different electric permittivity properties $\boldsymbol{\kappa}^{(\alpha)}$ ($\alpha = 1, 2$). The electric potential u^ε in Ω satisfies the Maxwell's equation in the quasi-static approximation in absence of free conduction currents in Ω_1^ε and Ω_2^ε, together with continuity of electric potential and normal component of electric displacement field across the interface Γ^ε.

$$\frac{\partial}{\partial x_j}\left(\kappa_{jl}^\varepsilon \frac{\partial u^\varepsilon}{\partial x_l}\right) = 0 \quad \text{in } \Omega \setminus \Gamma^\varepsilon, \tag{1a}$$

$$[\![u^\varepsilon]\!] = 0 \quad \text{on } \Gamma^\varepsilon, \tag{1b}$$

$$\left[\!\!\left[\kappa_{jl}^\varepsilon \frac{\partial u^\varepsilon}{\partial x_l} n_j\right]\!\!\right] = 0 \quad \text{on } \Gamma^\varepsilon, \tag{1c}$$

$$u^\varepsilon = \tilde{u} \quad \text{on } \partial\Omega, \tag{1d}$$

where n_j is the j-th component of unit normal vector to Γ^ε in the direction from Ω_1^ε to Ω_2^ε. The notation $[\![.]\!]$ is used to denote the jump of the enclosed function across the interface Γ^ε in the $\boldsymbol{n}$ direction. The function u_0 is prescribed on the boundary $\partial\Omega$.

Consider that the complex electric potential u^ε is given by $u^\varepsilon = \varphi^\varepsilon + i\psi^\varepsilon$ with $i^2 = -1$, and that the components of the complex dielectric permittivity tensor $\boldsymbol{\kappa}^\varepsilon$ are $\kappa_{jl}^\varepsilon = \alpha_{jl}^\varepsilon + i\beta_{jl}^\varepsilon$ ($j, l = 1, 2$). The real functions α_{jl}^ε and β_{jl}^ε, are assumed to be piecewise differentiable, rapidly oscillating and εY-periodic in the local variable $\boldsymbol{y}$. For each $\boldsymbol{x} \in \Omega$, these functions are defined as $\alpha_{jl}^\varepsilon(\boldsymbol{x}) = \alpha_{jl}\left(\frac{\boldsymbol{x}}{\varepsilon}\right)$, and $\beta_{jl}^\varepsilon(\boldsymbol{x}) = \beta_{jl}\left(\frac{\boldsymbol{x}}{\varepsilon}\right)$. In addition, the following symmetry and positivity conditions are imposed,

$$\alpha_{jl}^\varepsilon = \alpha_{lj}^\varepsilon, \quad \beta_{jl}^\varepsilon = \beta_{lj}^\varepsilon \tag{2a}$$

$$\alpha_{jl}^\varepsilon(\mathbf{x})\, a_j a_l \geq \varkappa\, a_j a_j \tag{2b}$$

where $\varkappa > 0$ is a constant and $\boldsymbol{a} = (a_1, a_2)$ is an arbitrary real vector.

The complex dielectric problem (1a)-(1d) can be equivalently rewritten as two-coupled real partial differential equations

$$\frac{\partial}{\partial x_j}\left(\mathcal{A}_{jl}^\varepsilon \frac{\partial \boldsymbol{U}^\varepsilon}{\partial x_l}\right) = \mathbf{0} \quad \text{in } \Omega \setminus \Gamma^\varepsilon, \tag{3a}$$

$$[\![\boldsymbol{U}^\varepsilon]\!] = \mathbf{0} \quad \text{on } \Gamma^\varepsilon, \tag{3b}$$

$$\left[\!\!\left[\left(\mathcal{A}_{jl}^\varepsilon \frac{\partial \boldsymbol{U}^\varepsilon}{\partial x_l}\right) n_j\right]\!\!\right] = \mathbf{0} \quad \text{on } \Gamma^\varepsilon, \tag{3c}$$

$$\boldsymbol{U}^\varepsilon = \tilde{\boldsymbol{U}} \quad \text{on } \partial\Omega, \tag{3d}$$

where $\boldsymbol{U}^\varepsilon = (\varphi^\varepsilon, \psi^\varepsilon)^T$, $\tilde{\boldsymbol{U}} = (\tilde{u}_1, \tilde{u}_2)^T$ and $\mathbf{0} = (0, 0)^T$ is the null vector of $\mathbb{R}^2$. The matrix A_{jl}^ε has components

$$\mathcal{A}_{11}^\varepsilon = \boldsymbol{\alpha}^\varepsilon, \quad \mathcal{A}_{12}^\varepsilon = \mathcal{A}_{21}^\varepsilon = -\boldsymbol{\beta}^\varepsilon, \quad \mathcal{A}_{22}^\varepsilon = -\boldsymbol{\alpha}^\varepsilon, \tag{4}$$

where $\boldsymbol{\alpha}^\varepsilon$ and $\boldsymbol{\beta}^\varepsilon$ are 2×2 matrices with components α_{jl}^ε and β_{jl}^ε, respectively.

3. Asymptotic homogenization procedure

Following [9], an asymptotic solution of (3a)–(3d) is

$$\boldsymbol{U}^\varepsilon(\boldsymbol{x}) = \boldsymbol{U}^{(0)}(\boldsymbol{x}) + \varepsilon \boldsymbol{N}_k(y) \frac{\partial \boldsymbol{U}^{(0)}(\boldsymbol{x})}{\partial x_k}, \tag{5}$$

with

$$\boldsymbol{U}^{(0)}(\boldsymbol{x}) = \begin{pmatrix} \varphi^{(0)}(\boldsymbol{x}) \\ \psi^{(0)}(\boldsymbol{x}) \end{pmatrix}, \quad \boldsymbol{N}_k(\boldsymbol{y}) = \begin{pmatrix} w^k(\boldsymbol{y}) & g^k(\boldsymbol{y}) \\ \zeta^k(\boldsymbol{y}) & \xi^k(\boldsymbol{y}) \end{pmatrix}.$$

The 2×2 matrix of functions $\boldsymbol{N}_k(\boldsymbol{y})$ are Y-periodic solutions of the local problems

$$\frac{\partial}{\partial y_j}\left(\mathcal{A}_{jl} \frac{\partial \boldsymbol{N}_k}{\partial y_l} + \mathcal{A}_{jk}\right) = \mathbf{O} \quad \text{in } Y \setminus \Gamma, \tag{6a}$$

$$[\![\boldsymbol{N}_k]\!] = \mathbf{O} \quad \text{on } \Gamma, \tag{6b}$$

$$\left[\!\!\left[\left(\mathcal{A}_{jl} \frac{\partial \boldsymbol{N}_k}{\partial y_l} + \mathcal{A}_{jk}\right) n_j\right]\!\!\right] = \mathbf{O} \quad \text{on } \Gamma, \tag{6c}$$

$$\langle \boldsymbol{N}_k \rangle = \mathbf{O}, \tag{6d}$$

where $\mathbf{O}$ denotes the 2×2 null matrix and the angular brackets represents the volume average per unit length over the unit cell. In particular, the effective coefficients are given by

$$\widehat{\mathcal{A}}_{jk} = \left\langle \mathcal{A}_{jk}(\boldsymbol{y}) + \mathcal{A}_{jl}(\boldsymbol{y}) \frac{\partial \boldsymbol{N}_k(\boldsymbol{y})}{\partial y_l} \right\rangle. \tag{7}$$

The local problems defined in (6a)-(6d) for the unknown local functions ω^k, ζ^k, and for g^k and ξ^k, are equivalent through the transformation $\omega^k = \xi^k$ and $\zeta^k = -g^k$.

3.1. Isotropic case

Consider that $\alpha^{\varepsilon}_{jl} = \alpha^{\varepsilon}\delta_{jl}$ and $\beta^{\varepsilon}_{jl} = \beta^{\varepsilon}\delta_{jl}$, where α and β are piece-wise functions. Then, the local functions w^k,ζ^k and g^k, ξ^k are $Y-$periodic solutions of the following cell problems $\mathscr{I}^k$ $(k = 1, 2)$,

$$\Delta g^k = 0, \quad \Delta \xi^k = 0 \quad \text{in } Y \setminus \Gamma, \tag{8a}$$

$$[\![g^k]\!] = 0, \quad [\![\xi^k]\!] = 0 \quad \text{on } \Gamma, \tag{8b}$$

$$\left[\!\!\left[\left(\alpha\frac{\partial \xi^k}{\partial y_l} + \beta\frac{\partial g^k}{\partial y_l}\right) n_j\right]\!\!\right] = -[\![\alpha]\!]\, n_k \quad \text{on } \Gamma, \tag{8c}$$

$$\left[\!\!\left[\left(\beta\frac{\partial \xi^k}{\partial y_l} - \alpha\frac{\partial g^k}{\partial y_l}\right) n_j\right]\!\!\right] = -[\![\beta]\!]\, n_k \quad \text{on } \Gamma, \tag{8d}$$

$$\langle g^k \rangle = 0, \quad \langle \pi^k \rangle = 0. \tag{8e}$$

Furthermore, the related effective coefficients are

$$\widehat{\alpha}_{jk} = \left\langle \alpha^{\varepsilon}\delta_{jk} + \beta^{\varepsilon}\frac{\partial g^k}{\partial y_j} + \alpha^{\varepsilon}\frac{\partial \xi^k}{\partial y_j} \right\rangle, \tag{9}$$

$$\widehat{\beta}_{jk} = \left\langle \beta^{\varepsilon}\delta_{jk} - \alpha^{\varepsilon}\frac{\partial g^k}{\partial y_j} + \beta^{\varepsilon}\frac{\partial \xi^k}{\partial y_j} \right\rangle. \tag{10}$$

In particular, $\widehat{\alpha} = \widehat{\alpha}_{11} = \widehat{\alpha}_{22}$, $\widehat{\beta} = \widehat{\beta}_{11} = \widehat{\beta}_{22}$ and $\widehat{\alpha}_{jk} = \widehat{\beta}_{jk} = 0$ for $j \neq k$.

3.2. Solution of the local problem I^k

Let us consider a square lattice of inclusions of radius R and period equal to 1. Doubly-periodic harmonic function that satisfies the given interface conditions and the null average condition over the unit cell is sought. Then, the following infinite system of algebraic equations is obtained

$$\begin{aligned}&\big(\boldsymbol{I} + (-1)^{k+1}\chi_{\alpha}\boldsymbol{W}^k\big)\tilde{\boldsymbol{A}}^k + \big(\chi^{+}_{\beta\alpha}\boldsymbol{I} \\ &\quad + (-1)^{k+1}\chi^{-}_{\beta\alpha}\chi_{\alpha}\boldsymbol{W}^k\big)\tilde{\boldsymbol{B}}^k = (-1)^{k+1}\boldsymbol{V}^1,\end{aligned} \tag{11a}$$

$$\begin{aligned}&\big(\chi^{+}_{\beta\alpha}\boldsymbol{I} + (-1)^{k+1}\chi^{-}_{\beta\alpha}\chi_{\alpha}\boldsymbol{W}^k\big)\tilde{\boldsymbol{A}}^k \\ &\quad - \big(\boldsymbol{I} + (-1)^{k+1}\chi_{\alpha}\boldsymbol{W}^2\big)\tilde{\boldsymbol{B}}^k = (-1)^{k+1}\boldsymbol{V}^2.\end{aligned} \tag{11b}$$

where $\boldsymbol{I}$ denotes the infinite identity matrix, $\tilde{\boldsymbol{A}}^k = (\tilde{a}^k_1, \tilde{a}^k_3, \ldots)^T$, $\tilde{\boldsymbol{B}}^k = (\tilde{b}^k_1, \tilde{b}^k_3, \ldots)^T$, $a^k_q = \tilde{a}^k_q R^q/\sqrt{q}$, $b^k_q = \tilde{b}^k_q R^q/\sqrt{q}$, $\boldsymbol{V}^1 = (\chi_{\alpha}R, 0, \ldots)^T$, $\boldsymbol{V}^2 = (\chi^{-}_{\beta\alpha}R, 0, \ldots)^T$ and

$$\boldsymbol{W}^k = \begin{cases} (-1)^{k+1}\pi R^2, & p+q = 2 \\ \sum\limits_{p=1}^{\infty}{}^{o} \sqrt{pq}\,\eta^k_{pq} R^{p+q}, & p+q > 2, \end{cases}$$

with

$$\eta^k_{pq} = \begin{cases} (-1)^{k+1}\pi, & p+q = 2, \\ \frac{(p+q-1)!}{p!q!} S_{p+q}, & p+q > 2, \end{cases}$$

and S_j are the reticulated sums. The matrices $\boldsymbol{W}^k$ are real, symmetric and bounded, and consequently the classical results from the theory of infinite systems can be used to solve (11a)-(11b). Moreover,

$$\chi_{\alpha} = \frac{[\![\alpha]\!]}{\alpha^{(1)} + \alpha^{(2)}}, \quad \chi^{+}_{\beta\alpha} = \frac{\beta^{(1)} + \beta^{(2)}}{\alpha^{(1)} + \alpha^{(2)}} \quad \text{and}$$

$$\chi^{-}_{\beta\alpha} = \frac{[\![\beta]\!]}{\alpha^{(1)} + \alpha^{(2)}}.$$

4. Results and discussion

Here we consider a composite with dissipative constituents, i.e. $\beta^{(1)} > 0$ and $\beta^{(2)} > 0$, and study the LE properties of the homogenized material. That is, the goal is to obtain $\hat{\beta}$ such that

$$\hat{\beta} > max(\beta^{(1)}, \beta^{(2)}). \tag{12}$$

The dual process of GE arising from active constituents induce to an equivalent scenario [7]. In [7], the following sufficient condition for LE was found,

$$\begin{cases} \lim\limits_{V_2 \to 0} \dfrac{\mathrm{d}\hat{\beta}}{\mathrm{d}V_2} > 0 & \text{if } \beta^{(1)} \geq \beta^{(2)}, \\ \lim\limits_{V_2 \to \frac{\pi}{4}} \dfrac{\mathrm{d}\hat{\beta}}{\mathrm{d}V_2} < 0 & \text{if } \beta^{(1)} \leq \beta^{(2)}. \end{cases} \tag{13a}$$

From (13a), LE is guaranteed for all values of $\beta^{(1)} > 0$ and $\beta^{(2)} > 0$ when $\beta_1 = \beta_2$.

Using the results of the previous sections the effective real and imaginary parts of the effective dielectric coefficient are given by

$$\widehat{\alpha} = \alpha^{(1)} - (-1)^{k+1}2\pi\left(\alpha^{(1)}a^k_1 + \beta^{(1)}b^k_1\right), \tag{14a}$$

$$\widehat{\beta} = \beta^{(1)} - (-1)^{k+1}2\pi\left(\beta^{(1)}a^k_1 - \alpha^{(1)}b^k_1\right). \tag{14b}$$

Following [6], we found short-formulas for $\hat{\alpha}$ and $\hat{\beta}$, by truncating the infinite system (11a)-(11b), i.e.

$$\begin{pmatrix} \tilde{\boldsymbol{A}}^k_{n_0} \\ \tilde{\boldsymbol{B}}^k_{n_0} \end{pmatrix} = \left((-1)^{k+1}\boldsymbol{\theta}\mathcal{I}_{n_0} + \mathcal{W}^k_{n_0}\right)^{-1} R\boldsymbol{e}_{2n_0}, \tag{15}$$

where the sub-index $n_0 \in \mathbb{N}$ represents the truncation order of the vectors $\tilde{\boldsymbol{A}}$, $\tilde{\boldsymbol{B}}$ and $\boldsymbol{e}$, and the matrices $\mathcal{I}$ and $\mathcal{W}^k$, which are given by

$$\mathcal{I} = \begin{pmatrix} \boldsymbol{I} & \boldsymbol{\Theta} \\ \boldsymbol{\Theta} & \boldsymbol{I} \end{pmatrix} \quad \text{and} \quad \mathcal{W}^k = \begin{pmatrix} \boldsymbol{W}^k & \boldsymbol{\Theta} \\ \boldsymbol{\Theta} & \boldsymbol{W}^k \end{pmatrix}. \tag{16}$$

Furthermore the matrix $\boldsymbol{\theta}$ is

$$\boldsymbol{\theta} = \begin{pmatrix} \theta_{11} & \theta_{12} \\ -\theta_{12} & \theta_{11}, \end{pmatrix} \tag{17}$$

where

$$\theta_{11} = \frac{\chi_{\alpha} + \chi^{-}_{\beta\alpha}\chi^{+}_{\beta\alpha}}{(\chi_{\alpha})^2 + (\chi^{-}_{\beta\alpha})^2} \quad \text{and} \quad \theta_{12} = \frac{\chi_{\alpha}\chi^{+}_{\beta\alpha} - \chi^{-}_{\beta\alpha}}{(\chi_{\alpha})^2 + (\chi^{-}_{\beta\alpha})^2}.$$

In [6], we also prove that the problems $\mathscr{I}^k$ $(k = 1, 2)$ are equivalent. Then, in the further analysis we set $k = 1$. Now, by fixing $n_0 = 3$ and identifying the components of the matrix $\boldsymbol{W}^1$ with w^1_{pq}, the linear system (15) is rewritten as

$$\begin{pmatrix}\tilde{a}_1^1\\ \tilde{a}_3^1\\ \tilde{a}_5^1\\ \tilde{b}_1^1\\ \tilde{b}_3^1\\ \tilde{b}_5^1\end{pmatrix} = \begin{pmatrix}\theta_{11}+w_{11}^1 & w_{13}^1 & w_{15}^1 & \theta_{12} & 0 & 0\\ w_{13}^1 & \theta_{11}+w_{33}^1 & w_{35}^1 & 0 & \theta_{12} & 0\\ w_{15}^1 & w_{35}^1 & \theta_{11}+w_{55}^1 & 0 & 0 & \theta_{12}\\ -\theta_{12} & 0 & 0 & \theta_{11}+w_{11}^1 & w_{13}^1 & w_{15}^1\\ 0 & -\theta_{12} & 0 & w_{13}^1 & \theta_{11}+w_{33}^1 & w_{35}^1\\ 0 & 0 & -\theta_{12} & w_{15}^1 & w_{35}^1 & \theta_{11}+w_{55}^1\end{pmatrix}^{-1} \begin{pmatrix}R\\ 0\\ 0\\ 0\\ 0\\ 0\end{pmatrix}. \tag{18}$$

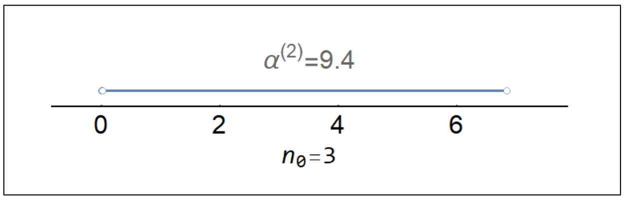

Figure 2. Domain $D = [0.025, 6.8]$ of $\beta^{(1)}$ where loss-enhancement properties are present for the effective material.

By solving the linear system (18) we find $\tilde{a}_1^1$ and $\tilde{b}_1^1$, and consequently, the effective coefficients given in (14a) and (14b). Expression (18) is useful in the analysis of LE properties since the sufficient conditions (13a) can be easily evaluated. Particularly, we consider a periodic composite where the dielectric properties of the cylinders are characterized by $\kappa^{(2)} = 9.4(1 + 0.006i)$ [8]. On the other hand, we assume that $\kappa^{(1)} = 1 + \beta^{(1)}i$ is the dielectric constant related to the matrix, and make a parametrical study by varying $\beta^{(1)}$ in such a way that LE properties are guaranteed in the effective material. In Fig. 2 we show the domain $D = [0.025, 6.8]$ in which loss-enhancement properties for the homogenized material is achieved. That is, when $\beta^{(1)} \in D$ the inequality (12) is valid. The number $V_p = \pi/4$ denotes the percolation limit where the cylinders are in contact. In Fig. 3 we show this fact by taking several values of $\beta^{(1)}$ in the interval D. It is noted that while we move from the left of the interval D to the right, the maximum value of the effective coefficient $\hat{\beta}$ move from the right to the left with respect to V_2 (volume fraction of the fibers). As it is remarked in [8], in low-loss periodic structures, the imaginary part of the effective dielectric constant is small as compared to its real part. From our analysis this result is reached for all fiber volumes in $[0, \pi/4]$ when $\beta^{(1)} \leq \alpha^{(1)}$ (see Fig. 4). However, in the domain D where LE properties are guaranteed, we found that $max(\hat{\beta}) < max(\hat{\alpha})$. For instance, we show this fact by taking the end point of the interval D (see Fig. 5).

5. Conclusions

In this work, closed-form formulas for the real and imaginary parts of effective coefficients of complex dielectric composites are derived. The analytical formulas obtained are used to estimate composites whose macroscopic answer exceeds those of the individual constituents. These results may be of interest in the context of metamaterials as in [8] where a similar composite was studied.

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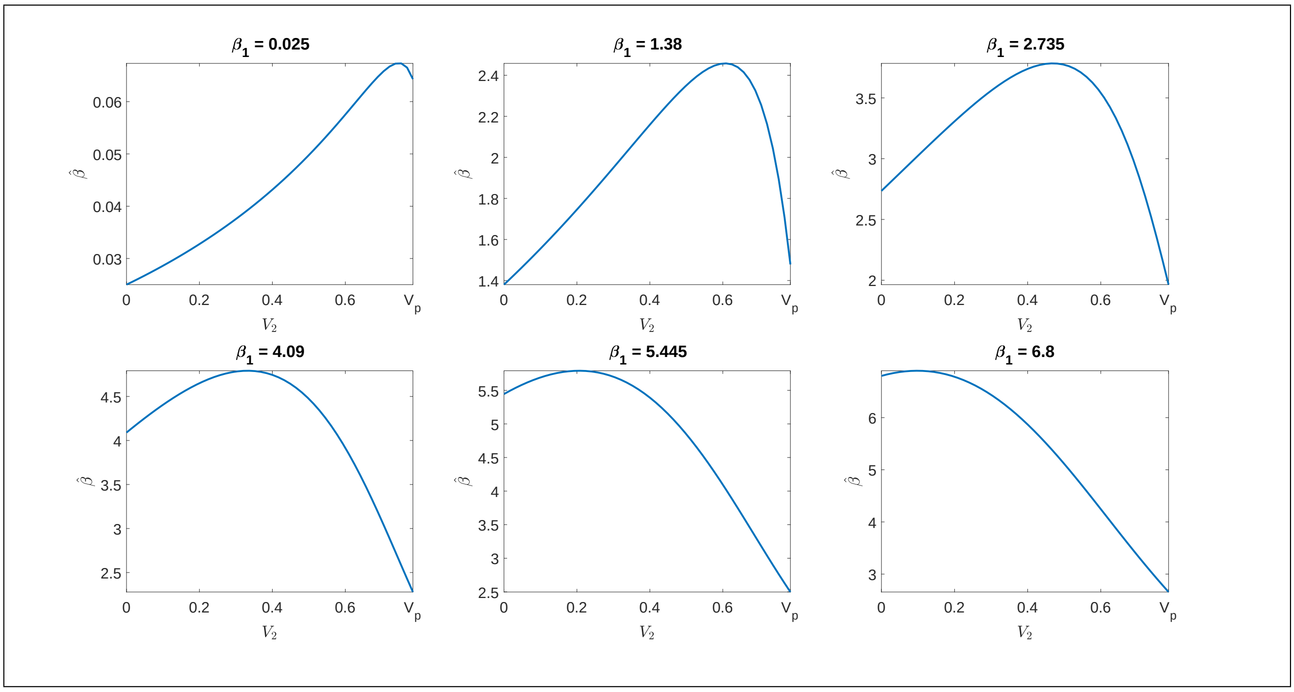

Figure 3. Imaginary part of the effective dielectric coefficient plotted for $\beta^{(1)}$ spanning six equal space points of the interval D with respect to fiber's volume fraction.

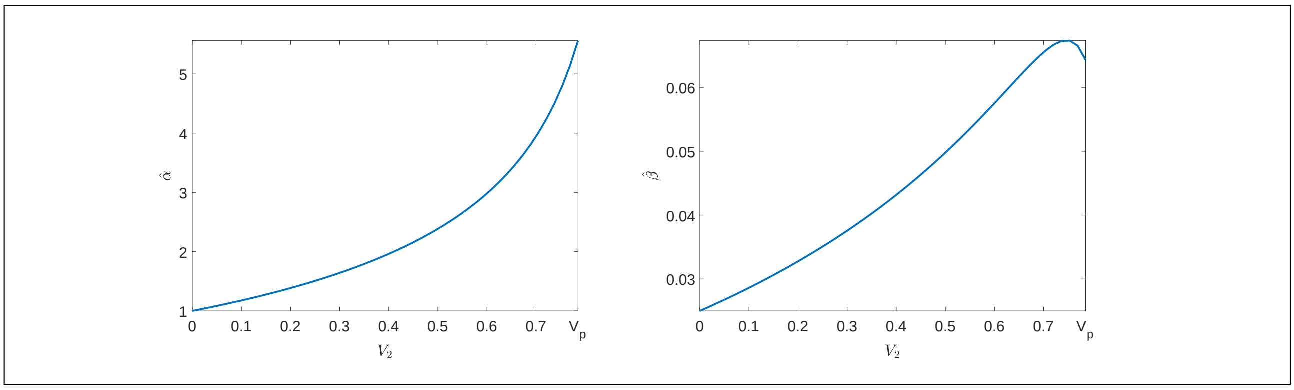

Figure 4. Note that $\hat{\alpha} << \hat{\beta}$ for $\kappa^{(1)} = 1 + 0.025i$ and $\kappa^{(2)} = 9.4 + 0.0564i$.

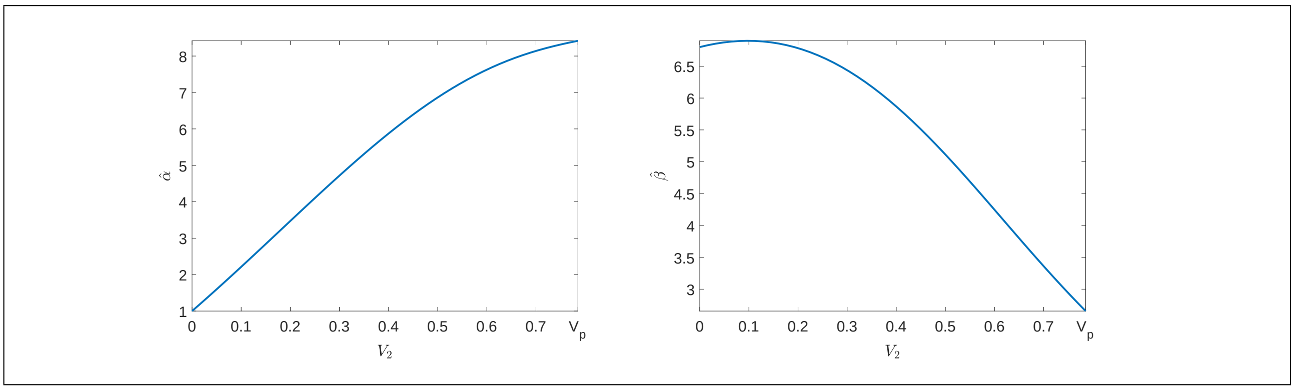

Figure 5. Here $max(\hat{\beta}) < max(\hat{\alpha})$ for $\kappa^{(1)} = 1 + 6.8i$ and $\kappa^{(2)} = 9.4 + 0.0564i$.